



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 21 28 29 30 31 32 33 34 35 36 37 38

ring nodes :

1 2 3 4 5 6 22 23 24 25 26 27

chain bonds :

1-10 2-13 3-14 4-7 5-12 6-11 7-8 7-9 8-21 15-16 15-18 16-17 22-31 23-34 24-35  
25-28 26-33 27-32 28-29 28-30 29-36 36-37 37-38

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27

exact/norm bonds :

7-8 7-9 28-29 28-30

exact bonds :

1-10 2-13 3-14 4-7 5-12 6-11 8-21 15-16 15-18 16-17 22-31 23-34 24-35 25-28 26-33  
27-32 29-36 36-37 37-38

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS  
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS 22:Atom  
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS  
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS

fragments assigned product role:

containing 22

fragments assigned reactant/reagent role:

containing 1

containing 15